Towards a Deep Microscopic Understanding of Ferroelectric Alloys

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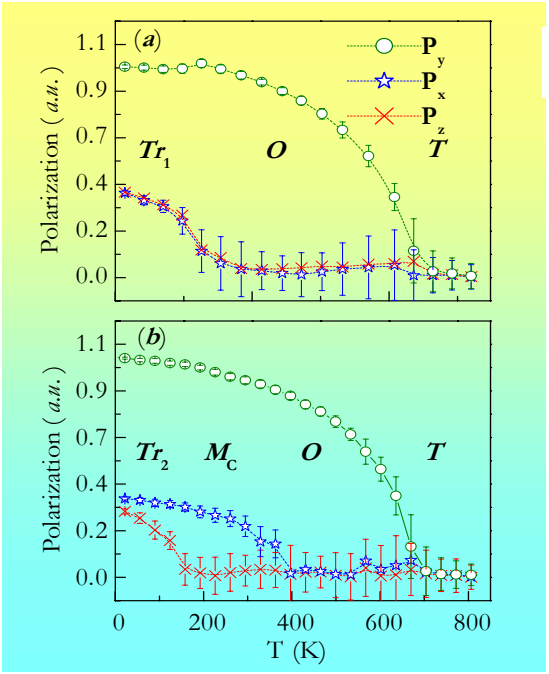
- Predicting the properties of novel compounds using ab-initio methods *is a must* to determine what materials might be of interest to efficiently guide the discovery of compounds with new or phenomenal properties.
- We studied ferroelectric superlattices made of different layers of lead zirconate titanate (PZT) with different titanium compositions (e.g., 44% and 52% of Ti) and with different *n* periods.
- Some superlattices exhibit new structural phases. These phases create an even larger piezoelectric response than the one occurring in the corresponding disordered material.
- Moreover, we found that superlattices can be "stuck" in a higher energy state than the ground state, which implies that the commonly used and assumed statistical laws are not always valid.



Polarization and corresponding phases as a function of temperature for PZT superlattices. T, O and M_C refer to tetragonal, orthorhombic and monoclinic phases, respectively. Tr_1 and Tr_2 are two different triclinic phases.

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Education:

- 1 undergraduate, 7 graduate students and 2 research associates contributed to this work.
- David Sichüga received his Master in Fall 2002

Outreach:

The graduate student sponsored by the grant (Aaron George) participated in an outreach activity in Fort Smith high schools in the Fall 2002. More precisely, Aaron was a judge in the BEST robotics competition. It was a competition between regional (Arkansas and surrounding states) high school and middle school students to promote science and engineering among local youth. Among the points on which the students were judged on were use of science and engineering process in robot construction and design, teamwork, presentation and sportsmanship.